Washington
TRU Solutions LLC

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October 4, 2004

Mr. M. Rahimi, Project Manager
NMSS/SFPO, Mail Stop O13D13
U.S. Nuclear Regulatory Commission
One White Flint North
11555 Rockville Pike
Rockville, MD 20852-2738

Subject: APPLICATION FOR REVISION 21 OF THE TRUPACT-II SHIPPING PACKAGE, DOCKET NO. 71-9218, AND REVISION 4 OF THE HalfPACT SHIPPING PACKAGE, DOCKET NO. 71-9279

Dear Mr. Rahimi:

Washington TRU Solutions LLC, on behalf of the U.S. Department of Energy (DOE), hereby submits Revision 21 to the application for a Certificate of Compliance (CoC) for the TRUPACT-II Packaging, U.S. Nuclear Regulatory Commission (NRC) Docket No. 71-9218, and Revision 4 to the application for a CoC for the HalfPACT Packaging, NRC Docket No. 71-9279. The application consists of the following documents:

- *TRUPACT-II Safety Analysis Report* (SAR), *Revision 21*
- *HalfPACT SAR, Revision 4*
- *Contact-Handled Transuranic Waste Authorized Methods for Payload Control* (CH-TRAMPAC), *Revision 2*
- *CH-TRU Payload Appendices, Revision 1.*

These document revisions request the authorization of TRUPACT-II shipments of high-wattage contact-handled transuranic (CH-TRU) waste under specific conditions and controls. The application includes revisions to CH-TRU Payload Appendix 6.12, Use of TRUPACT-II for the Shipment of High-Wattage CH-TRU Waste, to extend the methodology previously approved for approximately 2,000 containers of high-wattage CH-TRU waste from Technical Area 54 at Los Alamos National Laboratory (LANL). The proposed revisions allow the methodology to be applied to the shipment of high-wattage CH-TRU waste from any DOE site. The shipment of high-wattage CH-TRU waste from the Savannah River Site is proposed using a reduced G value provided that a high-dose criterion based on waste stream-specific data is met.

This application is crucial to the DOE complex in providing a safe and compliant path forward for the shipment of high-wattage CH-TRU waste without the need for repackaging. Repackaging high-wattage waste increases worker exposures at the DOE sites and is inconsistent with the ALARA principle, which requires that risk to workers be “as low as reasonably achievable.” In addition, several DOE sites are currently managing high-wattage CH-TRU waste inventories in aboveground storage configurations, which pose potential security risks. Approval of this application will assist the DOE sites in meeting site cleanup and closure milestones. For example, this application would allow the Savannah River Site, which has a closure milestone of 2006, to ship approximately 3,000 drums of high-wattage CH-TRU waste that are otherwise not shippable without repackaging.

The CH-TRAMPAC has been reformatted into the format used for the TRUPACT-II and HalfPACT SARs. Changes associated with the reformatting of the document are not indicated by redlining ("|") in the margin of the document. Only changes that constitute content that has not been previously approved by the NRC are indicated by redlining. Minor editorial revisions, as outlined in Attachment B, have also been made to the HalfPACT SAR, the CH-TRAMPAC, and the CH-TRU Payload Appendices.

This letter includes the following attachments:

- Attachment A — Enclosures to Letter
- Attachment B — Abstract of Application
- Attachment C — References
- Attachment D — Revised Documents.

As noted in previous application submittals, an NRC/DOE agreement exists to waive applicable review fees.

If you have any questions regarding this submittal, please contact Ms. J. A. Biedscheid at (505) 878-1343 or me at (505) 234-7463.

Sincerely,

MJ Caviness

M. L. Caviness, Manager
Packaging Engineering

BAD:clm

Attachments

cc: (without attachments)
M. A. Italiano, CBFO

September 2004

ATTACHMENT A

ENCLOSURES TO LETTER

Attachment B	Abstract of Application for Revision 21 of the TRUPACT-II Shipping Package, Docket No. 71-9218, and Revision 4 of the HalfPACT Shipping Package, Docket No. 71-9279
Attachment C	References
Attachment D	Revised Documents (One hard copy and seven CDs in Adobe PDF format)

ATTACHMENT B

ABSTRACT OF APPLICATION FOR REVISION 21 OF THE TRUPACT-II SHIPPING PACKAGE, DOCKET NO. 71-9218, AND REVISION 4 OF THE HalfPACT SHIPPING PACKAGE, DOCKET NO. 71-9279

The changes comprising the application for Revision 21 of the TRUPACT-II Shipping Package, Docket No. 71-9218, and Revision 4 of the HalfPACT Shipping Package, Docket No. 71-9279, include the following:

TRUPACT-II Safety Analysis Report:

The revision number and date have been revised to reflect the current application.

HalfPACT Safety Analysis Report:

The following revisions have been made to the HalfPACT Safety Analysis Report:

- The revision number and date have been revised to reflect the current application.
- Section 3.5.3 (page 3.5-3) has been revised to correct the HAC fire temperature readings reference from Table 3.5-3 to Table 3.5-5 and the associated packaging temperatures section number reference from Section 3.5.5 to Section 3.5.3 of the TRUPACT-II SAR.
- Section 6.4.3.4 (page 6.4-8) has been revised to remove the TDOP references from Case C, as the TDOP is not an authorized payload container for the HalfPACT.
- Section 6.4.3.5 (page 6.4-9) has been revised to remove the TDOP entries in the FGE limit summary table, as the TDOP is not an authorized payload container for the HalfPACT.

CH-TRAMPAC:

The CH-TRAMPAC has been reformatted into the format used for the TRUPACT-II and HalfPACT SARs. Editorial changes associated with the reformatting of the document are not indicated by redlining ("│") in the margin of the document. Only changes that constitute content that has not been previously approved by the NRC are indicated by redlining. In addition, the following revisions have been made to the CH-TRAMPAC:

- The revision number and date have been revised to reflect the current application.
- List of CH-TRU Payload Appendices (page xiv) has been revised to update the title of Appendix 6.12 to "Use of TRUPACT-II for the Shipment of High-Wattage CH-TRU Waste."
- Section 1.1 (page 1.1-1) has been revised to reflect the revised scope of Appendix 6.12.
- Section 2.1.1 (page 2.2-1) has been revised to clarify that empty 55-gallon drum(s) can be used as dunnage container(s) to complete a payload of pipe overpacks.
- Table 3.1-1 (page 3.1-4) has been revised to clarify TDOP entries in the FGE limit summary table, as the TDOP is not an authorized payload container for the HalfPACT.
- Section 5.0 (page 5.1-1) has been revised to specify that compliance with the gas generation requirements for Content Codes SQ 154 and SR 154, in addition to Content Code LA 154, is described in CH-TRU Payload Appendix 6.12.

- Section 6.1 (page 6.1-1) has been revised to specify that compliance with the payload certification requirements for Content Codes SQ 154 and SR 154, in addition to Content Code LA 154, is described in CH-TRU Payload Appendix 6.12.

CH-TRU PAYLOAD APPENDICES:

The following revisions have been made to the CH-TRU Payload Appendices:

- The revision number and date have been revised to reflect the current application.
- Table of Contents (page ii) has been revised to update the title of Appendix 6.12 to "Use of TRUPACT-II for the Shipment of High-Wattage CH-TRU Waste."
- Appendix 2.2, Procedure for Determining Numeric Payload Shipping Category (page 2.2-9), has been revised to correct a typographical error in the resistance factor for the SWB overpack with a filter type of 7.4 x 10^{-6} moles/second/mole fraction.
- Appendix 3.9, Determination of Steady-State VOC Concentrations from DACs (page 3.9-18), has been revised to correct a typographical error in the equation for Y_{ICL}.
- Appendix 3.10, Determination of Flammable Gas/Volatile Organic Compound Concentrations by Measurement, has been revised to correct typographical errors in Equations (5) and (6) (page 3.10-3) and Equation (20) (page 3.10-6).
- Appendix 6.12, Use of TRUPACT-II for the Shipment of High-Wattage CH-TRU Waste, has been revised to extend the methodology previously approved for approximately 2,000 containers of high-wattage CH-TRU waste from Technical Area 54 at Los Alamos National Laboratory (LANL). The proposed revisions allow the methodology to be applied to the shipment of high-wattage CH-TRU waste from any DOE site. The shipment of high-wattage CH-TRU waste from the Savannah River Site is proposed using a reduced G value provided that a high-dose criterion based on waste stream-specific data is met. In addition, based on operational experience at LANL with the evacuation process, the limits for all content codes (including LA 154) have been calculated for a final evacuation pressure of 2 torr.

ATTACHMENT C

REFERENCES

The following reference is provided in support of the application for Revision 21 of the TRUPACT-II Safety Analysis Report (SAR), Revision 4 of the HalfPACT SAR, Revision 2 of the Contact-Handled Transuranic Waste Authorized Methods for Payload Control (CH-TRAMPAC), and Revision 1 of the CH-TRU Payload Appendices:

- Shaw Environmental, Inc., September 2004, *High-Dose Criterion for Flammable Gas G Values and Dose-Dependent Net Gas G Values for Contact-Handled Transuranic Wastes*, Shaw Environmental, Inc., Albuquerque, New Mexico.

High-Dose Criterion for Flammable Gas G Values and Dose-Dependent Net Gas G Values for Contact-Handled Transuranic Wastes

Prepared for
Washington TRU Solutions LLC
Carlsbad, New Mexico

Prepared by
Shaw Environmental, Inc.
Albuquerque, New Mexico

September 2004

1.0 Summary

Dose-dependent G values for flammable gas, based on a dose criterion of >0.012 watt*year, are currently established for use in the Contact-Handled Transuranic Waste Authorized Methods for Payload Control (CH-TRAMPAC) for contact-handled transuranic (CH-TRU) waste transportation. The purpose of this report is to extend this concept to high-wattage wastes (Waste Material Type III.1, Solid Organic Materials, with high loadings of Pu-239 and/or Pu-238) that meet a higher dose criterion (>1.2 watt*year). Based on a high-dose criterion, these high-wattage, wastes are eligible for the use of lower G values in calculating flammable gas limits. This report presents data that demonstrate that the concept of dose dependent G values can also be extended to net gas for use in pressure analysis. Based on the information presented in this report, the following matrix of G values is demonstrated for use for Waste Material Type III.1 containers.

Bounding Flammable and Net Gas G Values for TRU Wastes (Waste Material Type III.1)		
Dose Range	**Bounding Flammable Gas G Value (molecules/100 eV)**	**Bounding Net Gas G Value (molecules/100 eV)**
Low Dose (Dose ≤ 0.012 watt*year)	3.40 [a]	8.40 [a]
Intermediate Dose (0.012 watt*year < Dose ≤ 1.2 watt*year)	1.09 [a]	3.47
High Dose (Dose > 1.2 watt*year)	0.49	1.67

[a] Current G values established in CH-TRU Authorized Methods for Payload Control (CH-TRAMPAC) for use in calculating flammable gas limits.

The scope of the high-dose criterion (>1.2 watt*year) is for high-wattage wastes from Savannah River Site (SRS), as the values are supported by actual field data from high-wattage SRS drums.

2.0 Introduction

2.1 Background

Gas generation, concentration, and pressure during transport of transuranic (TRU) wastes are restricted as follows (Reference 1):

- The hydrogen generated must be limited to a molar quantity that would be no more than 5 percent by volume of the innermost layer of confinement (or equivalent limits for other flammable gases).
- The gases generated in the payload are controlled to maintain the pressure within the shipping package to below the acceptable design pressure of the package.

As discussed in Appendices 6.1, 6.5, and 6.6 of the CH-TRU Payload Appendices (Reference 2), the primary mechanism for potential gas generation in TRU wastes is radiolysis. Using the gas generation rates of flammable and net (total) gas due to radiolysis, compliance with the above restrictions may be determined. The gas generation potential of a waste material, or "G value", is defined as the number of molecules of gas generated per 100 electron volts (eV) of energy absorbed. For a waste container with contents of a given waste type, the applicable flammable and net gas G values may be used in establishing gas generation, concentration, and pressure limits.

The flammable and net gas G values currently authorized in the CH-TRAMPAC for Waste Material Type III.1, Solid Organic Materials (comprised of materials like paper, plastic, cellulose, etc.), are as follows:

- For flammable gas, a bounding G value of 3.4 is used when the dose (measure of energy absorbed) is less than or equal to 0.012 watt*year. For a dose greater than 0.012 watt*year, results of the matrix depletion program (MDP) summarized in Appendix 3.3 of the CH-TRU Payload Appendices show that gas generation rates decrease with increased dose and a G value of 1.09 is used (Reference 2).

- For net gas, a bounding G value of 8.4 is used for all cases.

2.2 Purpose and Scope

The purpose of this report is to establish effective (or bounding) flammable and net gas G values for high-wattage TRU wastes based on dose criteria. The data and analysis presented show that a further decrease in G value for flammable gas (i.e., lower than that currently in use) can be established when the dose exceeds 1.2 watt*year. In addition, this report establishes net gas G values based on dose criteria. A summary of both flammable and net gas G values is provided in this report for the following dose conditions:

- Low Dose: ≤0.012 watt*year (currently established in the CH-TRAMPAC for flammable and net gas G values)

- Intermediate Dose: >0.012 and ≤1.2 watt*year (currently established in the CH-TRAMPAC for flammable gas G value and established in this report for net gas G value)

- High Dose: >1.2 watt*year (established in this report for flammable and net gas G values).

As summarized above, the low-dose flammable and net gas G values and the intermediate-dose flammable gas G value are currently established in the CH-TRAMPAC and are not within the scope of this report. This report establishes the intermediate-dose net gas G value for all Waste Material Type III.1 containers. This report limits the scope of the high-dose criterion and the use of associated flammable and net gas G values to high-wattage wastes from SRS based on confirmatory data from sampling and analysis of actual SRS high-wattage waste containers.

3.0 Theoretical Considerations

Theoretical considerations of chemical structures for molecules, bond energies, and radiolysis show that flammable and net gas G values should decrease with increasing dose as the bonds in the vicinity of the radioactive material are dissociated. The discussion herein focuses on cellulose, which is a common matrix in Waste Material Type III.1 and, in general, is bounding for gas generation.

Cellulose $(C_6H_{10}O_5)_n$ is a "long-chain" polymer polysaccharide carbohydrate linear macromolecule consisting of monomeric units of beta-glucose. The chemical structure of cellulose is depicted in Figure 1. Cellulosic materials commonly present in TRU wastes include paper, cloth, wood, and Benelex, which is composed of wood fiber plus phenolic resin. Other commercial materials that contain cellulosics include cellophane, cellulose acetate (rayon, molded items, paints, coatings), and ethyl cellulose (paints and molded items).

The controlling factor in the behavior of materials such as cellulose under irradiation is the chemical structure. Chemical bonds are not broken randomly even though the excitation energy may exceed the bond dissociation energy. Energy may be absorbed at one location on a molecule and then transferred to another location on the molecule, which results in a break of the chemical bond at the new location.

Based on the cellulose chemical structure, the types of bonds and the bond energies required to dissociate the various bonds are listed in Table 1. Different bond dissociation energies are reported depending on the functional group and the source of the information. The last column of Table 1 presents average values of the various bond energies based on the cited references. These average values are used in the following discussion. Based on the types of bonds present, the gas products expected from the radiolysis of cellulose include carbon dioxide (CO_2), hydrogen (H_2), carbon monoxide (CO), and methane (CH_4). The number and percentage of bond types, the energy (from the last column of Table 1), and percentage of total energy required to dissociate the bond types in cellulose are presented in Table 2. The fact that a variety of gases are generated indicates that most, if not all, of the bonds in the cellulose molecule are susceptible to radiolytic dissociation. Hydrogen may be generated by the breaking of C-H and O-H bonds that allow the hydrogen atoms to recombine into the hydrogen gas molecule. As shown in Table 2, these bonds represent approximately 50% of the bonds and 46% of the energy required to completely breakdown a cellulose monomer. Thus, there should be an equal likelihood of breakage of the other two types of bonds (i.e., C-C and C-O). The fact that CO, CO_2, and CH_4 are produced indicates that the C-C and C-O bonds are also broken, and the matrix will eventually be depleted of all atoms of C, H, and O in the vicinity of the radioactive source. The matrix depletion phenomenon manifests on a gross scale as a continuous decrease in the flammable and net gas G values as a function of dose from initial maximum G values.

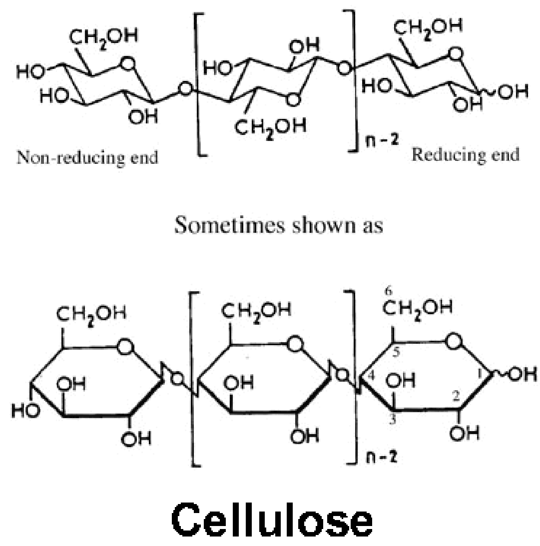

Figure 1. Chemical Structure of Cellulose

Table 1. Dissociation Energies for Bond Types in Cellulose

Bond Type	Bond Dissociation Energy (kcal/mole)			
	(Reference 3)	(Reference 4)	(Reference 5)	Average Value[a]
O-H	102	102	100-102 (alcohols)	102
C-H	80	81	91-99 (alkanes)	85
C-C	145	-	78-84 (alkanes)	113
C-O	70	-	89-90 (alcohols)	80

[a] The average value is calculated from the value reported from Reference 3, Reference 4, and the midpoint from Reference 5.

Table 2. Number and Percentage of Bond Types and Energy and Percentage of Total Energy Required to Dissociate Bond Types in Cellulose

Bond Type	Number per Cellulose Monomer	Percentage of Total Bonds	Energy Required (kcal/mole)	Percentage of Total Energy
O-H	3	14.3	306	15.7
C-H	7	33.3	595	30.6
C-C	5	23.8	565	29.0
C-O	6	28.6	480	24.7
Total	21	100.0	1946	100.0

4.0 Literature Review of Radiolysis Experiments for Net Gas

Numerous radiolysis experiments conducted in the past have demonstrated that, in addition to flammable gas G values, net gas G values also decrease with increasing dose. Details of these experiments are presented in Section 3.1.4.3.1 of Appendix 3.1 of the CH-TRU Payload Appendices (Reference 2) for cellulose. A summary of the relevant data is presented below.

Kazanjian measured gas consumption and generation from Pu-238 alpha irradiation of both wet and dry Kimwipes (paper tissues). The G values decreased as the dose increased. The net gas G value decreased from ~1.1 initially to ~0.5 at 6.0E23 eV for dry Kimwipes, and from ~0.6 initially to ~0.3 at an absorbed dose of 4.5E23 eV for wet Kimwipes. All G values were significantly lower for wet Kimwipes compared to the values for dry Kimwipes. This is attributed to some of the alpha decay energy being absorbed by water rather than by the cellulose.

Zerwekh also performed alpha radiolysis experiments on dry and wet mixtures of cellulosic materials. The dry mixture consisted of paper wipes, paper tissues, embossed paper towel with polyethylene backing, cheesecloth, and cotton laboratory smock material. The net gas G values for dry cellulosic materials decreased to approximately half of the initial values after about 750 days at an absorbed dose of 1.2E25 eV.

Bibler conducted alpha radiolysis experiments using a 5-M nitric acid Cm-244 solution, which was absorbed by paper tissue that was dried and folded to surround the Cm-244 deposit. A net gas G value of 1.9 was measured during the first five hours of one experiment, with the first measurement taken at an absorbed dose of ~4E19 eV. The net gas G value decreased to a value of 0.6 at an absorbed dose of 2.5E23 eV. Three different concentrations of Cm-244, with up to a factor of 4 difference, were used in the experiments, and all observations appeared to fit the same curve of decreasing net gas G value versus absorbed dose.

Kosiewicz measured net gas G values for paper of ~1.9 at very low absorbed dose and ~1.5 at a total absorbed dose of ~5E23 eV. The net gas G value decreased to half its initial value after an absorbed dose of ~2.5E24 eV. One set of experiments on paper was conducted in an argon atmosphere to measure the initial net gas G value at low dose. Data points were reported at absorbed dose as low as ~0.5E23 eV for 0.016 Curie of Pu-238 per gram of waste. A net gas G value of 1.4 was estimated. A similar experiment with air as the initial atmosphere reached a maximum net gas G value of 1.4 at ~4E23 eV. The first measured net gas G value was approximately 30% lower than the maximum value.

The cellulose net gas G value of 10.2 (which equates to an effective net gas G value of approximately 8.4 based on 82% of the energy being released from the plutonium particles [Appendix 3.2 of the CH-TRU Payload Appendices] [Reference 2]) currently used in all net gas calculations is based on gamma radiolysis experiments conducted by Ershov under conditions in which the oxygen was either absent or depleted. This net gas G value is approximately four units higher than any other experimentally determined value. Other cellulose radiolysis experiments conducted under an oxygen depleted regime measured initial net gas G values ranging from 0.5 to less than or equal to 6. Irradiation experiments conducted when oxygen was present yielded net gas G values ranging from 0.6 to 6.2.

In summary, investigations of radiolytic gas generation have repeatedly demonstrated that this process is a function of dose. While the above discussion focuses on selected studies for cellulose, similar experiments for other materials are documented in Appendix 3.1 of the CH-TRU Payload Appendices (Reference 2).

5.0 Analysis of Gas Generation Rate Data

Gas generation data from hundreds of CH-TRU waste containers and MDP test cylinder data were analyzed to derive both effective flammable and net gas G values as a function of dose. This section describes the data sets and analyses specific to Waste Material Type III.1, Solid Organic Materials, containers with doses of >0.012 watt*year.

5.1 Test Category Containers Gas Generation Test Data

The test category containers under this data set consist of:

- Flammable gas generation rate data from the testing of 268 55-gallon drums of CH-TRU waste (Waste Material Type III.1) from the Rocky Flats Environmental Technology Site (RFETS).

- Flammable gas generation rate data from the testing of 541 containers of Waste Material Type III.1 drums that have been disposed of at Waste Isolation Pilot Plant (WIPP) (obtained from the WIPP Waste Information System [WWIS], which is a computerized data management system used to gather, store, and process information pertaining to CH-TRU waste destined for or disposed of at the WIPP). For a portion of the 541 containers, net gas generation rate data from testing were also available.

For the analyses of this data set, the dose was calculated for each drum using the decay heat of the drum at the time of gas generation testing and the difference in years between gas generation testing and drum closure (i.e., generation).

An effective flammable gas G value was calculated for each drum from the following equation derived in the CH-TRAMPAC and CH-TRU Payload Appendices (References 1 and 2):

$$\text{Flammable gas } G_{eff} = \frac{CG * N_A * 100 * 1.602 \times 10^{-19} \text{ watt sec/eV}}{Q} \qquad (1)$$

where,

CG	=	Flammable gas generation rate obtained through gas generation testing (mole/second)
N_A	=	Avogadro's number (6.023E23 molecules/mole)
Q	=	Decay heat of drum (watt)

For the drums in this data set for which net gas generation rate data were available, the net gas effective G value for each drum was also obtained from Equation (1) by replacing the CG term with the net gas generation rate obtained through gas generation testing (mole/second).

For the other drums in this data set, the net gas effective G value was calculated for each drum using the ratio of the net to flammable gas G values for the bounding material for net gas generation (i.e., cellulose) when the established dose criteria of >0.012 watt*year has not been met. When dose is less than or equal to 0.012 watt*year, the effective net gas G value of cellulosics is 82% of 10.2 (8.364) at room temperature (70^{o}F) and the effective flammable gas G value is 82% of 3.2 (2.624) (References 1 and 2). Based on the theoretical arguments presented in Section 3.0 and additional analysis of the MDP experimental data, the net gas G value was scaled by the same factor that the flammable gas G value is reduced when the dose criterion of >0.012 watt*year is satisfied. Thus, the dose-dependent net gas G value (i.e., when dose >0.012 watt*year) may be calculated as follows:

$$^{\text{Dose-Dependent}}\text{Net gas }G_{\text{eff}} = {}^{\text{Dose-Dependent}}\text{Flammable gas }G_{\text{eff}} * \frac{8.364\text{ molecules net gas/100eV}}{2.624\text{ molecules flammable gas/100eV}} \quad (2)$$

5.2 SRS High-Wattage Drums Gas Generation Measurement Data

Flammable gas data on 247 high-wattage 55-gallon drums of CH-TRU waste (Waste Material Type III.1) from SRS were analyzed. The flammable gas generation rate was calculated for each drum using the measured flammable gas concentrations, the packaging configurations of the drums, and the time history of the drums through analytical solutions of the mass balance equations as described in Appendix 3.10 of the CH-TRU Payload Appendices (Reference 2). For each drum, the dose was calculated at the time of flammable gas measurement as the difference in years between measurement and drum closure and the reported decay heat of the drum. An effective flammable gas G value was calculated for each drum using Equation (1). The net gas G value was calculated for each drum using Equation (2).

5.3 Matrix Depletion Program Gas Generation Data for Net Gas

The MDP quantified the flammable gas G value for several waste matrices as a function of dose. However, the earlier study did not quantify net gas G values. The data available from the MDP test cylinder data were used to calculate the net gas effective G values as:

$$\text{Net gas }G_{\text{eff}} = \frac{\text{Flammable gas }G_{\text{eff}}}{\text{Mole fraction Flammable gas in Test Cylinder}} \quad (3)$$

6.0 Analysis of Dose-Dependent G Values

As summarized in Section 5.0, gas generation data were analyzed to derive both flammable and net gas G values for three sets of data for Waste Material Type III.1 containers with doses >0.012 watt*year. The data indicate that a further classification can be made for containers that have a dose >1.2 watt*year. Therefore, three dose ranges (low, intermediate, and high) for flammable and net gas G values are applicable. The low-dose range is appropriate for containers in which the absorbed dose is less than or equal to 0.012 watt*year. The intermediate-dose range is defined by an absorbed dose greater than 0.012 watt*year and less than or equal to 1.2 watt*year. The high-dose range is defined by absorbed doses greater than 1.2 watt*year. The flammable and net gas G values for the low-dose range have been established in previous efforts and are currently authorized (References 1 and 2). The flammable gas G value for the intermediate range was also established in previous efforts and documented in the CH-TRAMPAC and CH-TRU Payload Appendices (References 1 and 2). However, the net gas G value for dose >0.012 watt*year was not quantified and the low dose net gas G values were used (References 1 and 2). No separate G values for high dose have been previously established. The derivation of the G values for the intermediate-dose range (net gas only) and high-dose range (flammable and net gas) are summarized in the following sections.

*6.1 Intermediate-Dose Range (0.012 Watt*Year < Dose ≤ 1.2 Watt*Year)*

The mean, median, and 95% upper tolerance limit (UTL) values for flammable and net gas G values for Waste Material Type III.1 data summarized in Sections 5.1, 5.2, and 5.3 are presented in Table 3 for containers with an intermediate dose (i.e., 0.012 watt*year < dose ≤ 1.2 watt*year).

Table 3. Waste Material Type III.1 Flammable and Net Gas G Values Statistics for 0.012 Watt*Year < Dose ≤ 1.2 Watt*Year

Statistic	Flammable Gas G Value (molecules/100 eV)	Net Gas G Value (molecules/100 eV)
Mean Value	0.23	0.73
Median Value	0.08	0.27
95% UTL Value	0.96	3.05

For intermediate-dose range, the currently established flammable gas G value of 1.09 is retained (compared to 0.96 from Table 3). Using Equation (2) and a flammable gas G value of 1.09, the net gas G value obtained is 3.47 (compared to 3.05 from Table 3). The 3.47 value is applicable to all Waste Material Type III.1 containers in the intermediate-dose range.

*6.2 High-Dose Range (Dose > 1.2 Watt*Year)*

The mean, median, and 95% UTL values for the flammable and net gas G values for Waste Material Type III.1 data summarized in Sections 5.1 and 5.2 are presented in Table 4 for containers meeting the high-dose criterion (i.e., >1.2 watt*year).

Table 4. Waste Material Type III.1 Flammable and Net Gas G Values Statistics for Dose > 1.2 Watt*Year

Statistic	Flammable Gas G Value (molecules/100 eV)	Net Gas G Value (molecules/100 eV)
Mean Value	0.09	0.34
Median Value	0.03	0.11
95% UTL Value	0.49	1.67

For containers in the high-dose range, the flammable gas G value of 0.49 in Table 4 is valid. For net gas, use of Equation (2) and a flammable gas G value of 0.49 (from Table 4) results in a net gas G value of 1.56. However, the conservative value of 1.67 from Table 5 is applicable.

7.0 Conclusions

Bounding flammable and net gas G values for three dose ranges are presented in Table 5. The flammable and net gas G values for dose less than or equal to 0.012 watt*year are based on established values (References 1 and 2). The flammable gas G value of 1.09 (for dose greater than 0.012 and less than or equal to 1.2 watt*year) was determined by experimental data in the MDP and is the value currently used (References 1 and 2). The net gas G value for the intermediate-dose range, which is established by this report, is based on scaling the net gas G value for low dose by the same factor as the reduction in the flammable gas G value if the 0.012 watt*year dose criterion is satisfied. Thus, a net gas dose-dependent G value for the intermediate-dose range of 3.47 is applicable. The net gas G value of 3.47 for the intermediate-dose range is greater than those reported by the MDP, theoretical arguments, and drum data. For the high-dose range established by this report (i.e., >1.2 watt*year), the flammable gas G value of 0.49 is valid, based on the 95% UTL of G values determined from drum data. A net gas G value of 1.67 is applicable for this population.

Table 5. Bounding Flammable and Net Gas G Values for TRU Wastes

Dose Range	Bounding Flammable Gas G Value (molecules/100 eV)	Bounding Net Gas G Value (molecules/100 eV)
Low Dose (Dose ≤ 0.012 watt*year)	3.40 [a]	8.40 [a]
Intermediate Dose (0.012 watt*year < Dose ≤ 1.2 watt*year)	1.09 [a]	3.47
High Dose (Dose > 1.2 watt*year)	0.49	1.67

[a] Current G values established in CH-TRU Authorized Methods for Payload Control (CH-TRAMPAC) for use in calculating flammable gas limits.

Specific data from high-wattage and high-dose (>1.2 watt*year) containers at SRS (192 containers of the 247 drums discussed in Section 5.2) support the application of reduced G values for containers meeting the high-dose criterion. These data are summarized in Appendix A.

Additionally, the concentration of flammable gas in the headspace of six high-wattage, high-dose drums from SRS was measured over a period of time. The headspace (i.e., the void volume between the rigid liner and the drum) of these drums was purged with pure nitrogen gas at the time of venting. Table 6 presents the dose received by the container at the time of venting and the calculated flammable gas generation rate and effective G value for each drum. The effective flammable gas G values range from one to three orders of magnitude below previously established values for initial (i.e., non-dosed) matrices. In all cases, the flammable gas concentration continues to decrease after an initial increase following the venting and purging when the flammable gas from the inner confinement layers is released into the headspace. The continuing decrease in hydrogen concentrations provides additional evidence that the waste matrix has been substantially depleted by radiolysis and that no significant generation of gas is occurring in these drums of high wattage and high dose.

Table 6. Gas Generation Data for Six CH-TRU High Wattage SRS Drums

Container ID	Decay Heat (watt)	Dates of Generation and Venting with Purging	Flammable Gas Concentration Inside Rigid Liner at time of venting (vol. %)	Dose (watt*year)	Calculated Flammable Gas Generation Rate (mole/sec)	Effective Flammable Gas G Value
SR513321	1.70	4/3/1980 1/26/2004	54.27	40.48	1.100E-8	0.062
SR513748	0.855	8/19/1980 1/20/2004	31.74	20.03	6.465E-9	0.073
SR511993	1.96	7/10/1980 1/16/2004	56.38	45.99	1.147E-8	0.057
SR526779	0.239	7/9/1985 11/20/2003	42.60	4.39	9.369E-9	0.378
SR520741	6.46	12/8/1983 3/17/2004	9.92	130.99	2.108E-9	0.003
SR510325	6.29	8/5/1980 3/16/2004	5.89	148.43	1.196E-9	0.002

Based on these confirmatory results for SRS high-wattage drums, the use of the high-dose criterion is proposed only for high-wattage wastes at SRS.

8.0 References

Reference 1. U.S. Department of Energy, "Contact-Handled TRU Waste Authorized Methods for Payload Control (CH-TRAMPAC)," U.S. Department of Energy Carlsbad Field Office, Carlsbad, New Mexico.

Reference 2. U.S. Department of Energy, "CH-TRU Payload Appendices," U.S. Department of Energy Carlsbad Field Office, Carlsbad, New Mexico.

Reference 3. Dean, J.A, 1999, Lange's Handbook of Chemistry, 15th Edition, McGraw-Hill, Inc., New York, New York.

Reference 4. Blanksby, S.J. and G.B. Ellison, 2003, Bond Dissociation Energies of Organic Molecules, Accounts of Chemical Res. 2003; 36(4) pp 255 – 263, American Chemical Society, Washington, D.C.

Reference 5. Lyman W.J., W. F. Reehl, and D. H. Rosenblatt, 1982, Handbook of Chemical Property Estimation Methods, American Chemical Society, Washington, D.C.

ANALYSIS OF GAS GENERATION DATA FROM SRS HIGH-WATTAGE DRUMS

Appendix A to report on

High-Dose Criterion for Flammable Gas G Values and Dose-Dependent Net Gas G Values for Contact-Handled Transuranic Wastes

Appendix A

Analysis of Gas Generation Data From SRS High-Wattage Drums

Flammable gas data on drums of high-wattage contact-handled transuranic (CH-TRU) waste (Waste Material Type III.1) from the Savannah River Site (SRS) were provided by SRS from the Vent and Purge Program. In the raw data provided by the SRS, a total of 247 of the drums had reported finite (i.e., greater than zero) decay heat and flammable gas concentration values. Based on the dose that the drums had attained at the time of venting and purging, 192 of the drums are classified as high-wattage and high-dose (>1.2 watt*year). Based on discussions with SRS staff, the drums have a maximum of six plastic bag layers, one of which is a liner bag, and an optional rigid drum liner. Prior to shipment, the rigid drum liner and drum lid are vented in accordance with the requirements of the Contact-Handled Transuranic Authorized Methods for Payload Control (CH-TRAMPAC). The shipping category of each drum is 30 0109 1018.

The flammable gas generation rate (FGGR) was calculated for each drum using the measured flammable gas (hydrogen plus methane) concentrations, the packaging configuration of the drum, and the time history of the drum through analytical solutions of the mass balance equations as described in Appendix 3.10 of the CH-TRU Payload Appendices (Reference 1). An example of the calculation of the flammable gas G values for the high-wattage SRS containers is provided here for drum SR610641.

The drum was generated on April 8, 1997, and the venting and purging including flammable gas measurement was performed on October 24, 2003, for a total elapsed time of 2,390 days. The hydrogen concentration within the intact rigid liner was measured to be 1,214 parts per million (ppm) and the methane concentration was measured as 75 ppm for a total flammable gas concentration of 1,288 ppm. Based on the methodology documented in Appendix 3.10 of the CH-TRU Payload Appendices (Reference 1), the FGGR of the drum was calculated to be 5.095E-11 mole/second. Thus, this FGGR value will yield a total flammable gas concentration of 1,288 ppm within the intact rigid liner of the sealed drum after 2,390 days of storage following closure.

For each drum, the dose was calculated at the time of flammable gas measurement as the difference in years between measurement and drum closure (i.e., generation) and the reported decay heat of the drum. The decay heat of the drum is 0.3728 watt. Thus, the dose attained by the drum at the time of venting and purging is 2.4 watt*year. The effective flammable gas G value was calculated for the container as:

$$\text{Flammable gas } G_{eff} = \frac{CG * N_A * 100 * 1.602 \times 10^{-19} \text{ watt sec/eV}}{Q}$$

where,

CG	=	Flammable gas generation rate (5.095E-11 mole/second)
N_A	=	Avogadro's number (6.023E23 molecules/mole)
Q	=	Decay heat of drum (0.3728 watt)

Thus, the flammable gas G value for this particular container is 0.00132 molecules flammable gas/100 eV.

A summary of the gas generation statistical parameters for these 192 high-wattage and high-dose (>1.2 watt*year) drums is provided in below. As shown, the analysis of these SRS high-wattage and high-dose containers supports the use of a flammable gas G value of 0.49 when dose is >1.2 watt*year.

Statistical Parameters on Flammable Gas G Values for High Dose Range (Dose > 1.2 watt*year) SRS Drums

Parameter	Flammable Gas G Value (molecules/100 eV)
Mean Value	0.05
Median Value	0.005
95% UTL Value	0.36

References

1. U.S. Department of Energy, CH-TRU Payload Appendices, U.S. Department of Energy, Carlsbad Field Office, Carlsbad, New Mexico.

APPENDIX D

REVISED DOCUMENTS
(One Hard Copy and Seven CDs in Adobe PDF Format)

- *TRUPACT-II Safety Analysis Report*, *Revision 21*
- *HalfPACT Safety Analysis Report, Revision 4*
- *Contact-Handled Transuranic Waste Authorized Methods for Payload Control* (CH-TRAMPAC), *Revision 2*
- *CH-TRU Payload Appendices, Revision 1.*